Ground states of the atoms H, He,..., Ne and their singly positive ions in strong magnetic fields: The high field regime

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(February 2, 2008)

The electronic structure of the ground and some excited states of neutral atoms with the nuclear charge numbers $1 \leq Z \leq 10$ and their single positive ions are investigated by means of our 2D mesh Hartree-Fock method for strong magnetic fields $0.5 \leq \gamma \leq 10000$. For $\gamma = 10000$ the ground state configurations of all the atoms and ions considered are given by fully spin-polarized configurations of single-electron orbitals with magnetic quantum numbers ranging from $m = 0$ to $m = -N + 1$ where N is the number of the electrons. Focusing on the fully spin polarized situation we provide critical values of the magnetic field strength for which crossovers with respect to the spatial symmetries of the ground state take place. It is found that the neutral atoms and singly charged positive ions with $2 \leq Z \leq 5$ have one fully spin-polarized ground state configuration whereas for $6 \leq Z \leq 10$ one intermediate fully spin-polarized configuration with an orbital of $2p_0$ type occurs.

I. INTRODUCTION

The behavior and properties of atoms in strong magnetic fields is a subject which has attracted the interest of many researchers. Partially this interest is motivated by the astrophysical discovery of strong fields on white dwarfs and neutron stars [1–3]. On the other hand, the competition of the diamagnetic and Coulomb interaction, characteristic for atoms in strong magnetic fields, causes a rich variety of complex properties which are of interest on their own.

Investigations on the electronic structure in the presence of a magnetic field appear to be quite complicated due to the intricate geometry of these quantum problems. Most of the investigations in the literature focus on the hydrogen atom (for a list of references see, for example, [4–7]). These studies provided us with a detailed understanding of the electronic structure of the hydrogen atom in magnetic fields of arbitrary strengths. As a result the absorption features of certain magnetic white dwarfs could be explained and this allowed for a modeling of their atmospheres (see ref. [8] for a comprehensive review of atoms in strong magnetic fields and their astrophysical applications up to 1994 and ref. [9] for a more recent review on atoms and molecules in external fields). On the other hand there are a number of magnetic white dwarfs whose spectra remain unexplained and cannot be interpreted in terms of magnetized atomic hydrogen. Furthermore new magnetic objects are discovered (see, for example, Reimers et al [10] in the course of the Hamburg ESO survey) whose spectra await to be explained. Very recently significant progress has been achieved with respect to the interpretation of the observed spectrum of the prominent white dwarf GD229 which shows a rich spectrum ranging from the UV to the near IR. Extensive and precise calculations on the helium atom provided data for many excited states in a broad range of field strengths [11]. The comparison of the stationary transitions of the atom with the positions of the absorp-

tion edges of the observed spectrum yielded strong evidence for the existence of helium in the atmosphere of GD229 [12].

For atoms with several electrons there are two decisive factors which enrich the possible changes in the electronic structure with varying field strength compared to the one-electron system. First we have a third competing interaction which is the electron-electron repulsion and second the different electrons feel very different Coulomb forces, i.e. possess different one particle energies, and consequently the regime of the intermediate field strengths appears to be the sum of the intermediate regimes for the separate electrons.

There exist a number of investigations on two-electron atoms in the literature (see ref. [11] and references therein). Focusing on systems with more than two electrons however the number of investigations is very scarce [13–19]. Some of them use the adiabatic approximation in order to investigate the very high field regime. These works contain a number of important results on the properties and structure of several multielectron atoms. Being very useful for high fields the adiabatic approach does hardly allow to describe the electronic structure with decreasing field strength: particularly the core electrons of multi-electron atoms feel a strong nuclear attraction which can be dominated by the external field only for very high field strengths. In view of this there is a need for further quantum mechanical investigations on multi-electron atoms, particularly in the intermediate to high-field regime.

The ground states of atoms in strong magnetic fields have different spatial and spin symmetries in the different regions of the field strengths. We encounter, therefore, a series of changes i.e. crossovers with respect to their symmetries with varying field stength. The simplest case is the helium atom which possesses two ground state configurations: the singlet zero- and low-field ground state $1s^2$ and the fully spin-polarized high-field ground state $1s2p_{-1}$. In the Hartree-Fock approximation the transition point between these configurations is given by the field strength $\gamma = 0.711$. (If not indicated otherwise we use in the following atomic units for all quantities. In particular, the magnetic field $\gamma = B/B_0$ is measured in units $B_0 = \hbar c/ea_0^2 = 2.3505{\cdot}10^5\mathrm{T} = 2.3505{\cdot}10^9\mathrm{G}$.) In previous works we have investigated the series of transitions of the ground state configurations for the complete range of field strengths for the lithium [18] and carbon [19] atoms as well as the ion Li^+ [18]. The evolution and appearence of these crossovers and the involved configurations become more and more intricate with increasing number of electrons of the atom. Currently the most complicated atomic system with a completely known sequence of ground state electronic configurations for the whole range of magnetic field strengths is the neutral carbon atom [19]. Its ground state experiences six crossovers involving seven different electronic configurations which belong to three groups of different spin projections $S_z = -1, -2, -3$ onto the magnetic field. This series of ground state configurations was extracted from results of numerical calculations for more than twenty electronic configurations selected via a detailed analysis on the basis of general energetical arguments. The picture of these transitions is especially complicated at relatively weak and intermediate fields. Due to this circumstance the comprehensive investigation of the structure of ground states of atoms is a complex problem which has to be solved for each atom separately. On the other hand, the geometry of the atomic wave functions is simplified for sufficiently high magnetic fields: Beyond some critical field strength the global ground state is given by a fully spin polarized configuration. This allows us to push the current state of the art and to study the ground states of the full series of neutral atoms and singly charged positive ions with $Z \leq 10$, i.e. the sequence H, He, Li, Be, B, C, N, O, F, Ne, in the domain of high magnetic fields. For the purpose of this investigation we define the high field domain as the one, where the ground state electronic configurations are fully spin polarized (Fully Spin Polarized (FSP) regime). The latter fact supplies an additional advantage for calculations performed in the Hartree-Fock

approach, because our one-determinantal wave functions are eigenfunctions of the total spin operator $\mathbf{S^2}$. Starting from the high-field limit we will investigate the electronic structure and properties of the ground states with decreasing field strength until we reach the first crossover to a partially spin polarized (PSP) configuration, i.e. we focus on the regime of field strengths for which fully spin polarized configurations represent the ground state.

II. METHOD

The numerical approach applied in the present work coincides with that of our previous investigations [17–19]. Refs. [7,17,18,20] contain some more details of the mesh techniques. We solve the electronic Schrödinger equation for the atoms in a magnetic field under the assumption of an infinitely heavy nucleus (see below for comments on finite nuclear mass corrections) in the (unrestricted) Hartree-Fock approximation. The solution is established in cylindrical coordinates (ρ, ϕ, z) with the z-axis oriented along the magnetic field. We prescribe to each electron a definite value of the magnetic quantum number m_μ. Each one-electron wave function Ψ_μ depends on the variables ϕ and (ρ, z) as follows

$$\Psi_\mu(\rho, \phi, z) = (2\pi)^{-1/2} e^{-im_\mu\phi} \psi_\mu(z, \rho) \tag{1}$$

where μ indicates the numbering of the electrons. The resulting partial differential equations for $\psi_\mu(z, \rho)$ and the formulae for the Coulomb and exchange potentials have been presented in ref. [20].

The one-particle equations for the wave functions $\psi_\mu(z, \rho)$ are solved by means of the fully numerical mesh method described in refs. [7,20]. The feature which distinguishes the present calculations from those described in ref. [20] is the method for the calculation of the Coulomb and exchange integrals. In the present work as well as in ref. [17–19] we obtain these potentials as solutions of the corresponding Poisson equation.

Our mesh approach is flexible enough to yield precise results for arbitrary field strengths. Some minor decrease of the precision appears in very strong magnetic fields. With respect to the electronic configurations possessing high absolute values of magnetic quantum numbers of outer electrons some minor computational problems arose also at lower field strengths. Both these phenomena are due to a big difference with respect to the binding energies $\epsilon_{B\mu}$ of one electron wave functions belonging to the same electronic configuration

$$\epsilon_{B\mu} = (m_\mu + |m_\mu| + 2s_{z\mu} + 1)\gamma/2 - \epsilon_\mu \tag{2}$$

where ϵ_μ is the one electron energy and $s_{z\mu}$ is the spin z-projection. The precision of our results depends, of course, also on the number of the mesh nodes and can be improved in calculations with denser meshes. Most of the present calculations are carried out on sequences of meshes with the maximal number of nodes being 65×65.

III. RELEVANT PROPERTIES IN THE HIGH FIELD REGIME

In this section we provide some qualitative considerations on the problem of the ground states of multi-electron atoms in the high field limit. These considerations present a starting point for the combined qualitative and numerical considerations given in the following section. At very high field strengths the nuclear attraction energies and HF potentials (which determine the motion along the z axis) are small

compared to the interaction energies with the magnetic field (which determines the motion perpendicular to the magnetic field and is responsible for the Landau zonal structure of the spectrum). Thus in the limit ($\gamma \to \infty$), all the one-electron wave functions of the ground state belong to the lowest Landau zones, i.e. $m_\mu \leq 0$ for all the electrons, and the system must be fully spin-polarized, i.e. $s_{z\mu} = -\frac{1}{2}$. For the Coulomb central field the one electron levels form quasi 1D Coulomb series with the binding energy $E_B = \frac{1}{2n_z^2}$ for $n_z > 0$, whereas $E_B(\gamma \to \infty) \to \infty$ for $n_z = 0$, where n_z is the number of nodal surfaces of the wave function crossing the z axis. In the limit $\gamma \to \infty$ the ground state wave function must be formed of the tightly bound single-electron functions with $n_z = 0$. The binding energies of these functions decrease as $|m|$ increases and, thus, the electrons must occupy orbitals with increasing $|m|$ starting with $m = 0$.

In the language of the Hartree-Fock approximation the ground state wave function of an atom in the high-field limit is a fully spin-polarized set of single-electron orbitals with no nodal surfaces crossing the z axis and with non-positive magnetic quantum numbers decreasing from $m = 0$ to $m = -N + 1$, where N is the number of electrons. For the carbon atom, mentioned above, this Hartree-Fock configuration is $1s2p_{-1}3d_{-2}4f_{-3}5g_{-4}6h_{-5}$ with $S_z = -3$. For the sake of brevity we shall in the following refer to these ground state configurations in the high-field limit, i.e. the configuration generated by the tightly bound hydrogenic orbitals $1s, 2p_{-1}, 3d_{-2}, 4f_{-3}, \ldots$, as $|0_N\rangle$. The states $|0_N\rangle$ possess the complete spin polarization $S_z = -N/2$. Decreasing the magnetic field strength, we can encounter a series of crossovers of the ground state configuration associated with transitions of one or several electrons from orbitals with the maximal values for $|m|$ to other orbitals with a different spatial geometry of the wave function but the same spin polarization. This means the first few crossovers can take place within the space of fully spin polarized configurations. We shall refer to these configurations by mentioning, i.e. noting, only the difference with respect to the state $|0_N\rangle$. This notation can, of course, also be extended to non-fully spin polarized configurations. For instance the state $1s^2 2p_{-1}3d_{-2}4f_{-3}5g_{-4}$ with $S_z = -2$ of the carbon atom will be briefly refered to as $\left|1s^2\right\rangle$, since the default is the occupation of the hydrogenic series $1s, 2p_{-1}, 3d_{-2}, \ldots$ and only deviations from it are recorded by our notation.

In the following considerations we shall often refer to subsets of electronic states which possess different spin polarizations. As indicated above we will denote the set of electronic states with $S_z = -N/2$ as the FSP subset. Along with the global ground state it is expedient to consider also what we call local ground states which are the energetically lowest states with some definite degree of the spin polarization. For the purpose of the present work we need to know the local ground state of the subset of electronic states with $S_z = -N/2 + 1$ (which is the only partially spin polarized subset considered in this paper and which is refered to as subset PSP) in the high-field regime. This knowledge is necessary for the evaluation of the point of the crossover between the FSP and PSP ground states, i.e. for the determination of the critical field strengths at which the global ground state changes its spin polarization from $S_z = -N/2$ to $S_z = -N/2 + 1$. For sufficiently high fields the $\left|1s^2\right\rangle$ state is the local ground state of the PSP subset of electronic states.

IV. GROUND STATE ELECTRONIC CONFIGURATIONS IN THE HIGH-FIELD REGIME

Let us start with the high field limit and the state $|0_N\rangle$ and subsequently consider possible ground state crossovers which occur *with decreasing magnetic field strength*. In the high-field regime we have per definition only crossovers due to changes of the spatial orbitals and no spin-flip crossovers. According to the goals of the present work we investigate the possible global ground state configurations belonging to

the subset FSP and determine the transition points to the subset PSP. Since the detailed study of the latter subset of states for arbitrary field strengths goes beyond the scope of the present work we consider first only the $\left|1s^2\right\rangle$ state of this subset which is the local ground state of the subset PSP for sufficiently strong fields. Then we investigate the FSP ground states with decreasing field strength until we reach the point of crossover with the energy of the configuration $\left|1s^2\right\rangle$. Subsequently we need to consider other electronic configurations of the PSP set in order to determine the complete picture of the energy levels as a function of the field strength near the spin-flip crossover and, possibly, to correct the position of this point (the latter is necessary if the state $\left|1s^2\right\rangle$ is not the lowest one of the subset PSP at the spin-flip point).

Let us consider the ground state transitions within the subset FSP with decreasing field strength. The first of these transitions occurs when the binding energy associated with the outermost orbital ($m_N = -N + 1$) becomes less than the binding energy of one of the orbitals with $n_z > 0$. Due to the circumstance, that all the orbitals with $n_z > 0$ are not occupied in the high-field ground state configuration, it is reasonable to expect the transition of the outermost electron to one of the orbitals with $m = 0$ and either $n_z = 1$ (i.e. $2p_0$ orbital) or $n_z = 2$ (i.e. $2s$ orbital). The decision between these two possibilities cannot be taken on the basis of qualitative arguments. For the hydrogen atom or hydrogen-like ions in a magnetic field the $2p_0$ orbital is more strongly bound than the $2s$ orbital for any field strength. On the other hand, owing to the electronic screening of the nuclear charge in multi-electron atoms in field-free space the $2s$ orbital tends to be more tightly bound than the $2p_0$ orbital. Thus, we have two competing mechanisms and numerical calculations are required for the decision between the possible $|0_N\rangle - |2p_0\rangle$ and $|0_N\rangle - |2s\rangle$ crossovers to a new local FSP ground state. Our calculations for the $|2s\rangle$ state presented below in table VI for neutral atoms and in table X for positive ions show that the state $|2s\rangle$ becomes more tightly bound than the $|2p_0\rangle$ state only for rather weak field strengths, where this state cannot pretend to be the ground state of the corresponding atom or ion due to the presence of more tightly bound non-fully spin polarized states. In result the first intermediate ground state of the subset FSP, i.e. the state beside the $|0_N\rangle$ state which might be involved in the first crossover of the ground state with decreasing field strength, is the $|2p_0\rangle$ state. Calculations for the subset PSP (see below) show indeed, that this state is the global ground state in a certain regime of field strengths for the neutral atoms with $Z \geq 6$, i.e. C, N, O, F and Ne, as well as their positive ions C^+, N^+, O^+, F^+, Ne^+. For the atoms He, Li, Be and B ($Z \leq 5$) as well as for the ions Li^+, Be^+ and B^+ the state $\left|1s^2\right\rangle$ becomes more tightly bound than $|0_N\rangle$ for fields stronger that those associated with the $|0_N\rangle - |2p_0\rangle$ crossover and the $|2p_0\rangle$ never becomes the global ground state of these atoms and ions. Thus, both neutral atoms and positive ions A^+ with $Z \leq 5$ have only one fully spin polarized ground state configuration $|0_N\rangle$, which represents the global ground state above some critical field strength.

The question about a possible second intermediate fully spin polarized ground state occurring with further decreasing field strength arises for neutral atoms and positive ions with $Z \geq 6$ which possess the intermediate fully spin polarized ground state $|2p_0\rangle$. This state could be either a state, containing an additional orbital with $n_z = 1$ which would result in the $|2p_0 3d_{-1}\rangle$ configuration, or a state with an additional s-type orbital, i.e. $|2s2p_0\rangle$. The third possibility of the simultaneous transition of the electron with the magnetic quantum number $m_{N-1} = -N+2$ to the $3d_{-1}$ orbital and the electron in the $2p_0$ orbital to the $2s$ orbital, which gives the $|2s3d_{-1}\rangle$ configuration, can be excluded from the list of possible ground state configurations without a numerical investigation. The reason herefore is that the $3d_{-1}$ orbital is for any field strength more weakly bound than the $2p_0$ orbital and thus the $|2s2p_0\rangle$ configuration possess a lower energy than the $|2s3d_{-1}\rangle$ configuration for arbitrary magnetic field strengths. When comparing

the configurations $|2s2p_0\rangle$ and $|2p_03d_{-1}\rangle$ we can make use of what we have learned (see above) from the competing $|2p_0\rangle$ and $|2s\rangle$ configurations for higher field strengths: The $2s$ orbital is energetically preferable at weak magnetic fields whereas the $3d_{-1}$ orbital yields energetically lower configurations in the strong field regime. Thus, we perform calculations for the $|2p_03d_{-1}\rangle$ configuration for many field strengths and then perform at much fewer field strengths calculations to check the energy of the $|2s2p_0\rangle$ configuration in order to obtain the correct lowest energy and state of the set FSP.

The behavior of the energy levels described in the previous paragraph is illustrated in Figure 1. In this figure the energy curves for four possible fully spin polarized electronic configurations and two energy curves for the PSP subset of the neon ($Z = 10$) atom are presented. This figure shows, in particular, the energy curve of the high field ground state $|0_N\rangle$ which intersects with the curve $E_{|2p_0\rangle}(\gamma)$ at $\gamma = 159.138$. The latter energy remains the lowest in the FSP subset until the intersection of this curve with $E_{|2p_03d_{-1}\rangle}(\gamma)$ at $\gamma = 40.537$. This intersection occurs at higher field strength than the intersection of the curves $E_{|2p_0\rangle}(\gamma)$ and $E_{|1s^2\rangle}(\gamma)$ which is at $\gamma = 38.060$. On the other hand, the control calculations for the state $|2s2p_0\rangle$, not presented in Figure 1, show that its total energy for $\gamma = 38.060$ is larger than the energy $E_{|2p_03d_{-1}\rangle}$. According to the previous argumentation this means that the state $|2s2p_0\rangle$ is not the global ground state of the Ne atom for any magnetic field strengths. Furthermore the state $|2p_03d_{-1}\rangle$ is a candidate for becoming the global ground state of the neon atom in some bounded regime of the field strength. However, we have not yet performed (see below) a detailed investigation of the lowest energy curves of the PSP subset which is essential to take a definite decision on the global ground state configurations. For neutral atoms with $6 \leq Z \leq 9$ and positive ions A^+ with $6 \leq Z \leq 10$ the energies of the states $|2p_03d_{-1}\rangle$ and $|2s2p_0\rangle$ at the points of intersections of the curves $E_{|2p_0\rangle}(\gamma)$ and $E_{|1s^2\rangle}(\gamma)$ are higher than the energies of the states $|2p_0\rangle$ and $\left|1s^2\right\rangle$. This leads to the conjecture that no neutral atoms with $Z < 10$ and positive ions with $Z \leq 10$ can possess more than two different fully spin polarized ground state configurations in the complete range of field strengths.

The above concludes our considerations of the fully spin polarized ground state configurations. To prove or refute the above conjecture we have to address the question of the lower boundary of the fully spin polarized domain, i.e. the lowest field strength, at which a fully spin-polarized state represents the ground state of the atom considered. It is evident that this boundary value of the field strength is given by the crossover from a fully spin polarized to a non-fully spin polarized ground state with decreasing field strength.

First of all we have to check if the state $\left|1s^2\right\rangle$ has the lowest energy of all the states of subset PSP at the point of intersection of the curve $E_{|1s^2\rangle}(\gamma)$ with the corresponding energy curve for the local ground state configuration of subset FSP. Following our considerations for the fully spin polarized case we can conclude that calculations have to be performed first of all for the states $\left|1s^22p_0\right\rangle$ and $\left|1s^22s\right\rangle$.

The numerical calculations show, that for atoms with $Z \leq 6$ and ions with $Z \leq 7$, the state $\left|1s^2\right\rangle$ becomes the ground state while lowering the spin polarization from the maximal absolute value $S_z = -N/2$ to $S_z = -N/2 + 1$. For heavier atoms and ions we first remark that the state $\left|1s^2\right\rangle$ is not the energetically lowest one in the PSP subset at magnetic fields at which its energy becomes equal to the energy of the lowest FSP state. For these atoms and ions the state $\left|1s^22p_0\right\rangle$ lies lower than $\left|1s^2\right\rangle$ at these field strengths. One can see this behavior for the neon atom in Figure 1. The second possible PSP local ground state $\left|1s^22s\right\rangle$ (not presented in Figure 1) proves to be less tightly bound at these fields. These facts allow in the following a definite clarification of the picture of the global ground state configuration in the high field regime. For atoms with $Z \geq 7$ and positive ions with $Z \geq 8$ the intersection points between the state $\left|1s^22p_0\right\rangle$ and the energetically lowest state in the FSP subspace have to be calculated.

In result, the spin-flip crossover occurs at higher fields than this would be in the case of $\left|1s^2\right\rangle$ being the lowest state in the PSP subspace. In particular, the spin-flip crossover for the neon atom is found to be slightly higher than the point of the crossover $|2p_0\rangle - |2p_0 3d_{-1}\rangle$, and, therefore, this atom has in the framework of the Hartree-Fock approximation only two fully spin polarized configurations likewise other neutral atoms and positive ions with $6 \leq Z \leq 10$. The above conjecture is therefore refuted and the FSP $|2p_0 3d_{-1}\rangle$ represents never the global ground state configuration in the high field regime for all neutral atoms and positive ions with $Z \leq 10$. It should be noted that the situation with the neon atom can be regarded as a transient one due to closeness of the intersection $|2p_0\rangle - |2p_0 3d_{-1}\rangle$ to the intersection $|2p_0\rangle - \left|1s^2 2p_0\right\rangle$. This means that we can expect the configuration $|2p_0 3d_{-1}\rangle$ to be the global ground state for the sodium atom ($Z = 11$). In addition an investigation of the neon atom carried out on a more precise level than the Hartree-Fock method could also introduce some corrections to the picture described above.

After obtaining the new spin flip points for atoms with $7 \leq Z \leq 10$ and ions with $8 \leq Z \leq 10$ (which are transition points between the $|2p_0\rangle$ and $\left|1s^2 2p_0\right\rangle$ states) one has to check them with respect to the next (in the order of decreasing field strengths) possible PSP local ground state configurations. Analogously to the FSP subset these configurations are $\left|1s^2 2p_0 3d_{-1}\right\rangle$ and $\left|1s^2 2s 2p_0\right\rangle$. The numerical calculations show, that their energies lie higher than the energy of the $\left|1s^2 2p_0\right\rangle$ configuration at the spin flip points and they are therefore excluded from the list of the global ground states considered here.

The final picture of the crossovers of the global ground state configurations is presented in tables I (for the neutral atoms) and II (for the positive ions A^+). The corresponding values of the field strengths belonging to the point of crossover are underlined in these tables. The field strengths for other closelying crossovers which actually do not affect the scenario of the changes of the global ground state are also presented in these tables. In a graphical form these results are illustrated in Figures 2 (neutral atoms) and 3 (ions). Shown are the critical field strengths belonging to the crossovers of selected states of the atoms (ions) as functions of the nuclear charge. The filled symbols mark the crossovers of the energy levels which correspond to the actual transitions of the ground state configurations, whereas the analogous non-filled symbols correspond to magnetic field strengths of the crossovers not associated with changes in the ground state but excited states. One can see in these figures the dependencies of the field strengths for various types of crossovers on the charge of the nucleus. In particular, one can see many significant crossovers for $Z = 10$ lying very close from each other on the γ axis. This peculiarity in combination with the behavior of the curve $\gamma(Z)$ for the $|2p_0\rangle - |2p_0 3d_{-1}\rangle$ crossover allows one to expect the configuration $|2p_0 3d_{-1}\rangle$ to become a ground state configuration for $Z > 10$.

Some summarizing remarks with respect to the global ground state configurations in the high field regime are in order. The atoms and positive ions with $Z \leq 5$ have one ground state configuration $|0_N\rangle$. The atoms and ions with $6 \leq Z \leq 10$ possess two high field configurations. The C atom ($Z = 6$) plays an exceptional role in the sense that it is the only atom which shows the ground state crossover $|2p_0\rangle - \left|1s^2\right\rangle$ involving the $\left|1s^2\right\rangle$ state as a global ground state.

V. NUMERICAL RESULTS AND DISCUSSION

The tables III–X contain numerical values of the total energies of the neutral atoms and positive ions obtained in our Hartree-Fock calculations. Tables III, IV, V and VI contain the energies of the neutral atoms in the states $|0_N\rangle$, $|2p_0\rangle$, $\left|1s^2\right\rangle$ and $|2s\rangle$, respectively. The analogous results for the ions A^+ are

presented in tables VII, VIII, IX and X (the results are for the states $|0_N\rangle$, $|2p_0\rangle$, $\left|1s^2\right\rangle$ and $|2s\rangle$). The energies associated with the points of crossover for the global ground state both in neutral atoms and in their singly positive ions are presented in table XI. These energy values provide us with the ionization energies at the transition points. Being combined with the data of the previous tables they provide the behavior of the ionization energies of the atoms and the total energies of the atoms and positive ions in the complete high-field region.

In Figure 4 we present the ionization energies of neutral atoms divided by the ionization energy of the hydrogen atom as a function of the magnetic field strength. All the curves for multi-electron atoms at $\gamma < 600$ lie lower than the curve for hydrogen at the corresponding field strengths. But for $\gamma > 1500$ the ionization energies of all atoms exceed the ionization energy for the hydrogen atom. Moreover, with growing nuclear charge we observe a stronger increase of the ionization energy for stronger fields accompanied by a shift of the starting point for the growth to the regime of stronger magnetic fields. This strengthening of the binding of the multi-electron atoms at strong magnetic fields may be considered as a hint for increasingly favorable conditions for the formation of the corresponding negative ions.

Figure 5 presents the ionization energies for the $|0_N\rangle$ states for various field strengths depending on the nuclear charge Z, i.e. for all atoms H, He,..., Ne. All the field strengths presented in this figure are above the first crossover to another global ground state configuration. Thus, the ionization energies in this figure represent the differences between the energies of the high-field ground states of the neutral atoms and the corresponding singly charged positive ions. The curve for $\gamma = 2000$ can be considered as the prototype example for the general properties of the dependencies $E_{\rm Ion}(Z)$. For small values of Z this curve shows increasing values for $E_{\rm Ion}$ with increasing Z, then it has a maximum at $Z = 5$ and for $Z > 5$ it decreases with increasing Z. Analogous curves for lower field strengths have their maxima at lower values of Z. At $\gamma = 1000$ the ionization energy shows its maximal value at $Z = 2$, whereas the ionization energies for $\gamma = 500$ and $\gamma = 200$ decrease monotonically with increasing Z. On the other hand, for $\gamma = 5000$ and $\gamma = 10000$ we obtain a monotonically increasing behavior of the ionization energy for the whole range $1 \leq Z \leq 10$ of nuclear charges investigated in the present work. The behavior described above results from a competition of two different physical mechanisms which impact the binding energy of the outermost electron in the high-field ground state Hartree-Fock configuration. The first mechanism is the lowering of the binding energy of the outermost electron with increasing absolute value of its magnetic quantum number $|m|$ provided that this electron feels a constant nuclear charge. The latter assumption is a rough approximation to the case of relatively weak fields when the inner $Z - 1$ electrons screen more or less effectively the Coulomb field of the nucleus. The second and opposite tendency is associated with the decrease of the efficiency of this screening in extremely strong magnetic fields due to the fact that the geometry of the wave functions tends to be one-dimensional in these fields. In result the effect of increasing effective nuclear charge exceeds the effect of the growth of $|m|$ with increasing Z for the high-field ground state configurations. Continuing this qualitative consideration we point out that at each fixed γ the influence of the magnetic field on the inner electrons become less and less significant as Z increases which is due to the dominance of the Coulomb attraction potential of the nucleus over the magnetic field interaction. This has to result in a significant screening of the nuclear charge by these electrons. In result the functions $E_{\rm Ion}(Z)$ for strong fields defined on the whole interval $1 \leq Z < +\infty$ have maxima at some values for Z and decrease for sufficiently large values of Z.

Next we provide a comparison of the present results with adiabatic HF calculations which were carried out for multi-electron atoms in refs. [13,16]. We compare our results on the Hartree-Fock electronic structure of atoms in strong magnetic fields with results obtained by Neuhauser et al [13] via a one-

dimensional *adiabatic* Hartree-Fock approximation. The calculations in this work were carried out for the four field strengths $\gamma = 42.544$, $\gamma = 212.72$, $\gamma = 425.44$ and $\gamma = 2127.2$. For $Z \leq 9$ and all these field strengths and for $Z = 10$ at the three larger values of these fields the Hartree-Fock wave functions of the ground states are reported to be fully spin polarized with no nodes crossing the z axis. This conclusion differs from our result for $\gamma = 42.544$. According to our calculations at $\gamma = 42.544$ the wave functions without nodes crossing the z axis represent the ground states of atoms with $Z \leq 7$ (i.e. H, He, Li, Be, B, C and N) whereas for the atoms with $8 \leq Z \leq 10$ (i.e. O, F and Ne) the wave functions of the ground states are fully spin polarized with one nodal surface crossing the z axis. A numerical comparison of our results with those of refs. [13,16] is shown in table XII. All our values lie lower than the values of these adiabatic calculations. Since our total energies are upper bonds to the exact values we consider our HF results as being closer to the exact values compared to the results of the adiabatic HF calculations. Therefore, on the basis of our calculations combined with the results of [13,16] we can obtain an idea of the degree of the applicability of the adiabatic approximation for multi-electron atoms for different field strengths and nuclear charges. It is well known, that the precision of the adiabatic approximation decreases with decreasing field strength. The increase of the relative errors with decreasing field strength is clearly visible in the table. On the other hand, the relative errors of the adiabatic approximation possess the tendency to increase with growing Z, which is manifested by the scaling transformation $E(Z, \gamma) = Z^2 E(1, \gamma/Z^2)$ (e.g. [8,20]) well known for hydrogen-like ions. The behavior of the inner electrons is to some extent similar to the behavior of the electrons in the corresponding hydrogen-like ions. Therefore their behavior is to lowest order similar to the behavior of the electron in the hydrogen atom at magnetic field strength γ/Z^2 i.e. this behavior can be less accurately described by the adiabatic approximation at large Z values. The absolute values of the errors in the total energy associated with the adiabatic approximation are in many cases larger than the corresponding values of the ionization energies.

To conclude this section we discuss briefly three issues, which could affect the precision of the results presented above. These issues are electron correlations, effects due to the finite nuclear mass and relativistic corrections. For all these effects we have to distinguish between their influence on the total energy and on other quantities like the ionization energy and the field strength for the crossover of the energy levels. In most cases their influence on the latter values is much smaller due to the fact that they involve differences of total energies for quantum states possessing a similar atomic core. Let us start by addressing the problem of the electronic correlations which is the critical problem for the precision of the Hartree-Fock calculations. The final evaluation of the correlation effects is possible only on the basis of exact calculations going beyond the Hartree-Fock approximation. Therefore we can give here only qualitative arguments based on the geometry of the wave function and on existing calculations for less complicated systems. The dependence of the ratio of the correlation energy and the total binding energy for the two ground state configurations of the helium atom has been investigated in ref. [21]. This ratio for the $1s^2$ state decreases with growing γ from 1.4% at $\gamma = 0$ to about 0.6% at $\gamma = 100$. The same ratio for the $1s2p_{-1}$ state (high field ground state configuration) increases with growing γ. It remains however for all the field strengths considered essentially smaller the values for the $1s^2$ state. This result for the helium atom in strong magnetic fields allows us to speculate that for the field strengths considered here the correlation energy for atoms and positive ions heavier than helium atom does not exceed their corresponding values without fields. Due to the similar geometry of the inner shells in the participating electronic configurations we do not expect a major influence of the correlation effects both on the field strengths of the crossovers of the ground state configurations within the subsets FSP or PSP and on the ionization energies if the states of a neutral atom and the positive ion belong to the same subset. On

the other hand, the properties associated with configurations from different subsets (for instance values of the spin-flip crossover field strengths) can be affected more strongly by correlation effects.

Our second issue is the influence of the finite nuclear mass on the results presented above. A discussion of this problem is provided in ref. [11] and references therein. Importantly there exists a well-defined procedure which tells us how to relate the energies for infinite nuclear mass to those with a finite nuclear mass. The corresponding equations are exact for hydrogen-like systems and provide the lowest order mass corrections $O\left(\frac{m}{M}\right)$ (m and M are the electron and total mass, respectively) for general atoms/ions. Essentially they consist of a redefinition of the energy scale (atomic units $\longrightarrow$ reduced atomic units, due to the introduction of the reduced mass) and an additional energy shift $-(1/M_0)\gamma(M+S_z)$ where M_0 is the nuclear mass. The first effect can simply be 'included' in our results by taking the energies in reduced a.u. instead of a.u. The mentioned shift can become relevant for high fields. However, it can easily be included in the total energies presented here. We emphasize that it plays a minor role in the region of the crossovers of the ground state configurations and decreases significantly with increasing mass of the atom (nucleus).

Relativistic calculations for the hydrogen atom and hydrogen-like ions were performed by Lindgren and Virtamo [22] and Chen and Goldman [23]. Our considerations are based on the work by Chen and Goldman [23] which contains results for the $1s$ and $2p_{-1}$ states for a broad range of magnetic field strengths. Interpolating their results for the $1s$ state and using well known scaling transformations we can conclude that in the least favorable case of $Z = 10$ relativistic corrections $\delta E = (E^{\mathrm{relativistic}} - E^{\mathrm{non-relativistic}})/\,|E^{\mathrm{non-relativistic}}|$ have to be of the order $4 \cdot 10^{-4}$ for $\gamma = 200$ and $2 \cdot 10^{-4}$ for $\gamma = 10^4$. The relativistic corrections for the $2p_{-1}$ state at relatively strong fields appear to be of the same order of magnitude or smaller than for the $1s$ state. Thus, making a reasonable assumption that relativistic corrections for both inner and outer electrons are similar to those in the hydrogen-like ions with a properly scaled nuclear charge we can evaluate $|\delta E| \leq 4 \cdot 10^{-4}$ for $Z = 10$ and lesser for lower Z values. The same relative correction can be expected also for the ionization energies and energy values used for the determination of the crossovers of the electronic configurations.

VI. SUMMARY

In the present work we have applied our 2D Hartree-Fock method to the magnetized neutral atoms H, He, Li, Be, B, C, N, O, F and Ne in the high field regime which is characterized by fully spin-polarized electronic shells. Additionally we have studied the crossover from fully spin polarized to partially spin polarized global ground state configurations. The highest field strength investigated was $\gamma = 10000$. Our single-determinant Hartree-Fock approach supplies us with exact upper bounds for the total energy. A comparison with adiabatic calculations in the literature shows the decrease of the precision of the latter with growing Z.

The investigation of the geometry of the spatial part of the electronic wave function demonstrates that in the high-field limit this wave function is a composition of the lowest Landau orbitals with absolute values of the magnetic quantum number growing from $|m| = 0$ up to $|m| = N-1$, where N is the number of the electrons: i.e. we have the series $1s$, $2p_{-1}$, $3d_{-2}$,... For atoms with $2 \leq Z \leq 5$ these states of type $1s2p_{-1}3d_{-2}\ldots$ represent the complete set of the fully spin-polarized ground state configurations. Heavier atoms $6 \leq Z \leq 10$ have one intermediate ground state configuration associated with the low-field end of the fully spin polarized region. This state contains one $2p_0$ type orbital (i.e. the orbital with a negative

z parity and $|m| = 0$) instead of the orbital with the positive z parity and the maximal value of $|m|$. Extrapolating our data as a function of the nuclear charge Z we expect that a third fully spin polarized ground state configuration occurs first for $Z = 11$, i.e. the sodium atom. The third configuration is suggested to be the $|2p_0 3d_{-1}\rangle$ state. The critical field strength which provides the crossover from the partially spin polarized to the fully spin polarized regime depends sensitively on the changes of the geometry of the wave functions. Indeed a number of different configurations have been selected as candidates for ground states in the crossover regime and only concrete calculations could provide us with a final decision on the energetically lowest state of the non-fully spin polarized electronic states. Generally speaking all the spin-flip crossovers mentioned above involve a pairing of the $1s$ electrons, i.e. the pair of orbitals $1s^2$. The carbon atom ($Z = 6$) plays an exceptional role since it is the only neutral atom which possesses two fully spin polarized configurations and the $\left|1s^2\right\rangle$ as a global non-fully spin polarized ground state configuration. The spin-flip crossover of the carbon atom preserves the total magnetic quantum number. All other atoms N, O, F and Ne ($7 \leq Z \leq 10$) possess instead the $\left|1s^2 2p_0\right\rangle$ configuration as a non-fully spin polarized ground state for strong fields. We have determined the positions, i.e. field strengths, of the crossovers of the ground states. Beyond this total energies have been provided for many field strengths for several low-lying excited states.

An analogous investigation has been carried out for singly charged positive ions $2 \leq Z \leq 10$. The structure of the fully spin polarized ground state configurations for these ions is the following: The ions with $3 \leq Z \leq 5$ have one fully spin polarized ground state configuration analogous to the high-field limit of the neutral atoms. For $6 \leq Z \leq 10$, analogously to the neutral atoms, there exist two fully spin polarized ground state configurations. Depending on the values of the nuclear charge number Z the spin-flip transitions associated with the lowering of the spin polarization with decreasing field strength lead also to wave functions of different spatial symmetries. These data being combined with the data for neutral atoms allow us to obtain the ionization energies of the atoms. The dependencies of the ionization energies on the nuclear charge at fixed field strength generally exhibit maxima at certain values of Z. The positions of these maxima shift to larger values of Z with increasing field strength. We provide some qualitative arguments explaining this behavior of $E_{\mathrm{Ion}}(Z)$. Finally we have given some remarks on the interactions going beyond the present level of investigation, i.e. correlations and finite nuclear mass effects as well as relativistic corrections.

Acknowledgments

Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

[1] J. P. Ostriker and F. D. A. Hartwick, *Astrophys. J.* 153 (1968) 797.

[2] J. Trümper, W. Pietsch, C. Reppin, W. Voges, R. Stauben, and E. Kendziorra, *Astrophys. J.* 219 (1978) L105.

[3] J. D. Landstreet, in *Cosmical Magnetism*, edited by D. Lynden-Bell (Kluwer, Boston, 1994), p.55.

[4] W. Rösner, G. Wunner, H. Herold, and H. Ruder, *J. Phys. B* 17 (1984) 29.

[5] H. Friedrich and D. Wintgen, *Phys.Rep.* 183 (1989) 37.

[6] Yu.P. Kravchenko, M.A. Liberman and B. Johansson, *Phys.Rev.Lett.*77 (1996) 619.

[7] M. V. Ivanov, *J. Phys. B* 21 (1988) 447.

[8] H. Ruder, G. Wunner, H. Herold and F. Geyer, *Atoms in Strong Magnetic Fields*, Springer-Verlag 1994.

[9] *Atoms and Molecules in Strong External Fields*, edited by P. Schmelcher and W. Schweizer, Plenum Press New York and London (1998)

[10] D. Reimers, S. Jordan, V. Beckmann, N. Christlieb, L. Wisotzki, *Astr.& Astrophys.* 337 (1998) L13

[11] W. Becken, P. Schmelcher and F.K. Diakonos, *J. Phys. B* 32 (1999) 1557.

[12] S. Jordan, P. Schmelcher, W. Becken, and W. Schweizer, *Astr.&Astrophys.* 336 (1998) 33.

[13] D. Neuhauser, S. E. Koonin, and K. Langanke, *Phys. Rev. A* 33 (1986) 2084; 36 (1987) 4163.

[14] M. D. Jones, G. Ortiz, and D. M. Ceperley, *Phys. Rev. A.* 54 (1996) 219.

[15] E. Müller, *Astron. & Astrophys.* 130 (1984) 415

[16] M. Demeur, P.-H. Heenen, and M. Godefroid, *Phys. Rev. A* 49 (1994) 176.

[17] M. V. Ivanov, *Phys. Lett. A* 239 (1998) 72.

[18] M.V. Ivanov, P. Schmelcher, *Phys. Rev. A* 57 (1998) 3793.

[19] M.V. Ivanov, P. Schmelcher, acc. f. publ. in *Phys. Rev. A*

[20] M. V. Ivanov, *Optics and Spectroscopy* 70 (1991) 148; *J. Phys. B* 27 (1994) 4513.

[21] P.Schmelcher, M.V.Ivanov and W.Becken, *Phys.Rev.A* 59 (1999) 3424.

[22] K. A. U. Lindgren and J. T. Virtamo, *J. Phys. B* 12 (1979) 3465; J. T. Virtamo and K. A. U. Lindgren, *Phys. Lett. A* 71 (1979) 329.

[23] Z. Chen and S. P. Goldman, *Phys.Rev.A* 45 (1999) 1722.

Figure Captions

Figure 1. The total energies (in atomic units) of the relevant states of the neon atom under consideration for the determination of the ground state electronic configurations for the high field regime.

Figure 2. The magnetic field strengths (a.u.) corresponding to crossovers of energy levels in neutral atoms as functions of the nuclear charge. The filled symbols mark crossovers between global ground state configurations.

Figure 3. Same as Figure 2 but for the singly positive ions.

Figure 4. Ionization energies of neutral atoms divided by the ionization energy of the hydrogen atom as a function of the magnetic field strength (a.u.).

Figure 5. Ionization energies of the states $|0_N\rangle$ of the neutral atoms ($1 \leq Z \leq 10$) for different magnetic field strengths.

TABLE I. Magnetic field strengths γ (a.u.) for energy level crossovers in neutral atoms. Ground state crossovers are underlined.

Z	$\|0_N\rangle - \|1s^2\rangle$	$\|0_N\rangle - \|2p_0\rangle$	$\|2p_0\rangle - \|1s^2\rangle$	$\|2p_0\rangle - \|1s^2 2p_0\rangle$	$\|2p_0\rangle - \|2p_0 3d_{-1}\rangle$	$\|2p_0 3d_{-1}\rangle - \|1s^2\rangle$
2	0.711					
3	2.153					
4	4.567	2.529	4.765451			
5	8.0251	7.923	8.0325			
6	12.577	18.664	12.216			
7		36.849	17.318	17.398		
8		64.720	23.3408	23.985		
9		104.650	30.285	31.735	22.744	30.6125
10		159.138	38.151	40.672	40.537	38.060

TABLE II. Magnetic field strengths γ (a.u.) for energy level crossovers in positive ions A^+. Ground state crossovers are underlined.

Z	$\|0_N\rangle - \|1s^2\rangle$	$\|0_N\rangle - \|2p_0\rangle$	$\|2p_0\rangle - \|1s^2\rangle$	$\|2p_0\rangle - \|1s^2 2p_0\rangle$	$\|2p_0\rangle - \|2p_0 3d_{-1}\rangle$
3	2.0718				
4	4.501	1.464			
5	7.957	5.575			
6	12.506	14.536	12.351		
7		30.509	17.429		
8		55.747	23.434	23.849	
9		92.624	30.364	31.612	
10		143.604	38.220	40.559	33.353

TABLE III. Total energies (a.u.) of the high-field ground states $|0_N\rangle$ of neutral atoms in strong magnetic fields.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$
1	−0.69721056	−0.83116892	−1.0222139	−1.38039889	−1.74779718	−2.21539853	−3.01786074
2	−2.615551	−2.959690	−3.502051	−4.617251	−5.829513	−7.427704	−10.264493
3	−5.97052	−6.57080	−7.520029	−9.576936	−11.939018	−15.1626119	−21.05055
4	−10.80902	−11.72880	−13.16961	−16.30690	−20.01753	−25.232499	−35.00768
5	−17.1771	−18.45812	−20.46843	−24.83956	−30.06363	−37.55469	−51.91499
6	−25.1007	−26.7843	−29.4282	−35.18153	−42.07989	−52.08903	−71.6285
7	−34.5971	−36.7230	−40.0600	−47.3314	−56.06309	−68.81304	−94.0501
8	−45.6798	−48.2846	−52.3718	−61.2866	−72.005397	−87.7104	−119.112
9	−58.3588	−61.4777	−66.3692	−77.0449	−89.89720	−108.7661	−146.7620
10				−94.60624	−109.7289	−131.9650	−176.964
Z	$\gamma = 100$	$\gamma = 200$	$\gamma = 500$	$\gamma = 1000$	$\gamma = 2000$	$\gamma = 5000$	$\gamma = 10000$
1	−3.7898043	−4.7271451	−6.257088	−7.6624234	−9.3047652	−11.873419	−14.14097
2	−13.07665	−16.57908	−22.46665	−28.03209	−34.6989	−45.4246	−55.1514
3	−27.01927	−34.58499	−47.55830	−60.05892	−75.282411	−100.2482	−123.313
4	−45.10519	−58.08264	−80.67357	−102.75480	−129.9790	−175.2704	−217.695
5	−66.99699	−86.60738	−121.16488	−155.3296	−197.8655	−269.440	−337.230
6	−92.4552	−119.8127	−168.5248	−217.1413	−278.1612	−381.8097	−480.875
7	−121.3027	−157.4300	−222.3434	−287.65764	−370.2004	−511.536	−647.685
8	−153.405	−199.2455	−282.28330	−366.430	−473.413	−657.871	−836.767
9	−188.657	−245.085	−348.0593	−453.0748	−587.294	−820.140	−1047.3242
10	−226.976	−294.807	−419.430	−547.259	−711.4106	−997.7478	−1278.622

TABLE IV. Total energies (a.u.) of neutral atoms in strong magnetic fields in the fully spin polarized states $|2p_0\rangle$.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$	$\gamma = 100$	$\gamma = 200$
1	−0.224760	−0.260007	−0.297711	−0.347618	−0.382650	−0.413378	−0.445685	−0.463618	−0.476532
2	−2.477333	−2.730171	−3.130766	−3.953993	−4.842630	−6.00481	−8.05248	−10.072	−12.588
3	−5.969573	−6.492478	−7.324937	−9.125540	−11.17884	−13.96583	−19.0436	−24.1951	−30.734
4	−11.06254	−11.89891	−13.22133	−16.10812	−19.51207	−24.27725	−33.2000	−42.4440	−54.368
5		−19.05098	−20.92634	−25.03513	−29.94166	−36.95414	−50.377973	−64.5298	−83.031
6		−28.0195	−30.4938	−35.96012	−42.52774	−52.02820	−70.51870	−90.275	−116.4070
7		−38.8370	−41.9590	−48.9040	−57.29256	−69.5147	−93.6004	−119.5977	−154.272
8		−51.5182	−55.3413	−63.877	−74.2380	−89.4093	−119.592	−152.453	−196.522
9		−66.0734	−70.6514	−80.8826	−93.3580	−111.6968	−148.4508	−188.7802	−243.1024
10		−82.5108	−87.8960	−99.9271	−114.64655	−136.36054	−180.1312	−228.500	−293.944

TABLE V. Total energies (a.u.) of neutral atoms in strong magnetic fields in the states $\left|1s^2\right\rangle$.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$	$\gamma = 100$	$\gamma = 200$
2	−2.8144511	−2.688885	−2.289145	−0.532445	+3.110634	+11.319608	+38.14390	+85.00416	+181.10639
3	−7.58789	−7.666532	−7.662455	−6.942304	−4.617769	+1.705656	+24.97942	+68.17347	+159.57479
4	−14.82273	−15.16179	−15.57496	−15.91027	−15.04644	−10.97100	+7.83395	+46.25962	+131.4188
5	−24.5395	−25.20257	−26.11859	−27.59737	−28.27946	−26.68603	−13.06555	+19.65113	+97.1970
6	−36.7864	−37.8130	−39.3061	−42.06081	−44.38721	−45.44649	−37.57176	−11.36933	+57.3384
7	−51.5899	−53.0202	−55.1513	−59.3169	−63.4083	−67.27185	−65.5935	−46.5970	+12.1743
8	−68.967	−70.8400	−73.6672	−79.3704	−85.3599	−92.1817	−97.0777	−85.8840	−38.0379
9	−88.930	−91.2830	−94.8623	−102.2227	−110.2464	−120.1897	−131.9955	−129.1244	−93.0956
10	−111.491	−114.3575	−118.7427	−127.8738	−138.0661	−151.3018	−170.3322	−176.2422	−152.8395

TABLE VI. Total energies (a.u.) of neutral atoms in strong magnetic fields in the states $|2s\rangle$.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$	$\gamma = 100$
2	−2.452834	−2.649185	−2.998243	−3.76667	−4.62593	−5.7711	−7.8134	−9.8438
3	−6.047868	−6.480293	−7.188888	−8.88983	−10.91060	−13.69420	−18.8014	−23.9861
4	−11.23262	−11.99646	−13.14233	−15.78294	−19.12479	−23.89990	−32.9045	−42.2253
5	−18.1278	−19.24491	−20.95537	−24.62942	−38.19566	−36.35453	−49.9355	−64.243
6				−35.57332	−41.68450	−51.0639	−69.770585	−89.815
7				−48.6234	−56.2802	−68.08282	−92.3323	−118.778
8				−63.7371	−73.2021	−87.5117	−117.5887	−151.001
9				−80.8912	−92.4162	−109.4449	−145.5587	−186.4023
10				−100.0783	−113.8625	−133.92080	−176.2966	−224.937

TABLE VII. Total energies (a.u.) of the high-field ground states $|0_N\rangle$ of positive ions A^+ in strong magnetic fields.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$
2	−2.2346282	−2.4409898	−2.7888422	−3.5438677	−4.3901481	−5.5215956	−7.5463093
3	−5.640062	−6.114623	−6.894080	−8.629427	−10.651315	−13.4297434	−18.525475
4	−10.51258	−11.31312	−12.59206	−15.42817	−18.820184	−23.612005	−32.61959
5	−16.9017	−18.07243	−19.93091	−24.01520	−28.93504	−36.02020	−49.63544
6	−24.8433	−26.4227	−28.9235	−34.40433	−41.01061	−50.62785	−69.44195
7	−34.3550	−36.3826	−39.5839	−46.5957	−55.04672	−67.41737	−91.94699
8		−47.9633	−51.9215	−60.5880	−71.0369	−86.37441	−117.08457
9			−65.9423	−76.3802	−88.9723	−107.4850	−144.8061
10			−81.6509	−93.9710	−108.8443	−130.7348	−175.0743
Z	$\gamma = 100$	$\gamma = 200$	$\gamma = 500$	$\gamma = 1000$	$\gamma = 2000$	$\gamma = 5000$	$\gamma = 10000$
2	−9.5605466	−12.071443	−16.2898727	−20.2706955	−25.028351	−32.65713	−39.548989
3	−23.699944	−30.260769	−41.50393	−52.323018	−65.47657	−86.9940	−106.8134
4	−41.93414	−53.90638	−74.73619	−95.07513	−120.11947	−161.7052	−200.5709
5	−63.947265	−82.55711	−115.33672	−147.71743	−187.99221	−255.6619	−319.6394
6	−89.51120	−115.87500	−162.80039	−209.6030	−268.2990	−367.8817	−462.931
7	−118.45429	−153.5960	−216.7194	−280.1976	−360.3670	−497.502	−629.454
8	−150.6447	−195.5087	−276.7565	−359.0516	−463.6191	−643.7651	−818.311
9	−185.9795	−241.4411	−342.6284	−445.780	−577.553	−805.9918	−1028.687
10	−224.3773	−291.251	−414.09358	−540.0501	−701.7295	−983.5779	−1259.8444

TABLE VIII. Total energies (a.u.) of positive ions A^+ in strong magnetic fields in the fully spin polarized states $|2p_0\rangle$.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$	$\gamma = 100$	$\gamma = 200$
3	−5.450607	−5.790277	−6.354440	−7.6155748	−9.07498561	−11.052577	−14.60723	−18.1514	−22.5884
4	−10.71847	−11.39964	−12.50590	−14.969431	−17.896267	−21.986880	−29.579033	−37.35540	−47.2987
5	−17.58187	−18.62668	−20.31984	−24.06890	−28.57270	−35.01093	−47.26504	−60.06278	−76.6646
6	−26.2094	−27.6300	−29.9454	−35.09561	−41.30920	−50.308209	−67.773425	−86.30316	−110.6170
7	−36.6424	−38.4731	−41.4488	−48.10689	−56.17490	−67.94617	−91.12203	−116.03024	−149.0175
8			−54.8620	−63.1295	−73.19399	−87.94947	−117.30577	−149.19626	−191.75146
9				−80.1774	−92.3729	−110.32119	−146.3062	−185.7521	−238.7295
10				−99.2581	−113.7112	−135.0539	−178.0971	−225.6432	−289.8700

TABLE IX. Total energies (a.u.) of positive ions A^+ in strong magnetic fields in the states $\left|1s^2\right\rangle$.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$	$\gamma = 100$	$\gamma = 200$
3	−7.217983	−7.164014	−6.962999	−5.850510	−3.110916	+3.748961	+27.964647	+72.09337	+164.66867
4	−14.49163	−14.70591	−14.95181	−14.96820	−13.75773	−9.217910	+10.42836	+49.70820	+135.95916
5	−24.2429	−24.78674	−25.54108	−26.71999	−27.08417	−25.06410	−10.65835	+22.86883	+101.46468
6	−36.5110	−37.4273	−38.7685	−41.23663	−43.25931	−43.91255	−35.28670	−8.30098	+61.43184
7	−51.3324	−52.6586	−54.6467	−58.5397	−62.33918	−65.81095	−63.40519	−43.64463	+16.13450
8	−68.725	−70.500	−73.1912	−78.6347	−84.3435	−90.78611	−94.97381	−83.03149	−34.19097
9		−90.962	−94.412	−101.5242	−109.2779	−118.8537	−129.9684	−126.3622	−89.3511
10		−114.054	−118.316	−127.2092	−137.1413	−150.0207	−168.3763	−173.5637	−149.190

TABLE X. Total energies (a.u.) of the positive ions A^+ in strong magnetic fields in the states $|2s\rangle$.

Z	$\gamma = 0.5$	$\gamma = 1$	$\gamma = 2$	$\gamma = 5$	$\gamma = 10$	$\gamma = 20$	$\gamma = 50$	$\gamma = 100$
3	−5.482414	−5.725577	−6.125201	−7.168333	−8.489089	−10.34858	−13.7869	−17.2792
4	−10.88665	−11.48854	−12.39822	−14.49715	−17.22586	−21.18159	−28.68072	−36.4493
5	−17.83551	−18.82816	−20.35231	−23.60163	−27.76915	−34.02228	−46.19941	−59.0447
6		−27.9171	−30.0961	−34.69799	−40.35174	−49.03420	−66.40440	−85.0457
7				−47.83068	−55.11866	−66.30856	−89.28664	−114.3624
8				−62.9964	−72.1475	−85.93862	−114.84057	−146.90998
9				−80.1907	−91.4315	−108.01546	−143.08156	−182.6254
10				−99.4125	−112.9303	−132.5918	−174.0451	−221.4723

TABLE XI. Total energies (a.u.) of the neutral atoms and ions A^+ at the crossover points of the ground state configurations.

Z	γ	Atomic state(s)	$-E$(Atomic)	Ionic state(s)	$-E(A^+)$
2	0.711	$\|0_N\rangle$, $\|1s^2\rangle$	2.76940	$\|0_N\rangle$	2.32488
3	2.153	$\|0_N\rangle$, $\|1s^2\rangle$	7.64785	$\|0_N\rangle$	7.00057
	2.0718	$\|1s^2\rangle$	7.65600	$\|0_N\rangle$, $\|1s^2\rangle$	6.94440
4	4.567	$\|0_N\rangle$, $\|1s^2\rangle$	15.9166	$\|0_N\rangle$	15.07309
	4.501	$\|1s^2\rangle$	15.91625	$\|0_N\rangle$, $\|1s^2\rangle$	15.01775
5	8.0251	$\|0_N\rangle$, $\|1s^2\rangle$	28.18667	$\|0_N\rangle$	27.16436
	7.957	$\|1s^2\rangle$	28.17996	$\|0_N\rangle$, $\|1s^2\rangle$	27.10004
6	18.664	$\|0_N\rangle$, $\|2p_0\rangle$	50.9257	$\|0_N\rangle$	49.50893
	14.536	$\|2p_0\rangle$	47.23836	$\|0_N\rangle$, $\|2p_0\rangle$	45.77150
	12.351	$\|2p_0\rangle$	45.07386	$\|2p_0\rangle$, $\|1s^2\rangle$	43.72095
	12.216	$\|2p_0\rangle$, $\|1s^2\rangle$	44.9341	$\|1s^2\rangle$	43.70075
7	36.849	$\|0_N\rangle$, $\|2p_0\rangle$	84.4186	$\|0_N\rangle$	82.58182
	30.509	$\|2p_0\rangle$	79.34493	$\|0_N\rangle$, $\|2p_0\rangle$	77.41246
	17.429	$\|2p_0\rangle$	66.72786	$\|2p_0\rangle$, $\|1s^2\rangle$	65.26170
	17.398	$\|2p_0\rangle$, $\|1s^2 2p_0\rangle$	66.69306	$\|1s^2\rangle$	65.25362
8	64.720	$\|0_N\rangle$, $\|2p_0\rangle$	130.6806	$\|0_N\rangle$	128.4054
	55.747	$\|2p_0\rangle$	124.1125	$\|0_N\rangle$, $\|2p_0\rangle$	121.69825
	23.985	$\|2p_0\rangle$, $\|1s^2 2p_0\rangle$	94.3773	$\|2p_0\rangle$	92.78308
	23.849	$\|1s^2 2p_0\rangle$	94.3336	$\|2p_0\rangle$, $\|1s^2 2p_0\rangle$	92.62502
9	104.650	$\|0_N\rangle$, $\|2p_0\rangle$	191.8770	$\|0_N\rangle$	189.1446
	92.624	$\|2p_0\rangle$	183.6944	$\|0_N\rangle$, $\|2p_0\rangle$	180.7819
	31.735	$\|2p_0\rangle$, $\|1s^2 2p_0\rangle$	128.1605	$\|2p_0\rangle$	126.4414
	31.612	$\|1s^2 2p_0\rangle$	128.1125	$\|2p_0\rangle$, $\|1s^2 2p_0\rangle$	126.2897
10	159.138	$\|0_N\rangle$, $\|2p_0\rangle$	270.220	$\|0_N\rangle$	267.0112
	143.604	$\|2p_0\rangle$	260.2740	$\|0_N\rangle$, $\|2p_0\rangle$	256.8459
	40.672	$\|2p_0\rangle$, $\|1s^2 2p_0\rangle$	168.4734	$\|2p_0\rangle$	166.6327
	40.559	$\|1s^2 2p_0\rangle$	168.4217	$\|2p_0\rangle$, $\|1s^2 2p_0\rangle$	166.4863

TABLE XII. Absolute values of the total energies (keV) of the high-field ground states of neutral atoms in strong magnetic fields compared with the literature. $B_{12} = B/(10^{12}\mathrm{G})$.

	$B_{12}=0.1$			$B_{12}=0.5$		$B_{12}=1$		$B_{12}=2.3505$ ($\gamma=1000$)		$B_{12}=5$	
Z	IS ($\|2p_0\rangle$)	IS	NKL	IS	NKL	IS	NKL	IS	DHG	IS	NKL
1		0.07781	0.0761	0.13114	0.130	0.16222	0.161	0.20851	0.206	0.25750	0.2550
2		0.26387	0.255	0.46063	0.454	0.57999	0.574	0.76279	0.754	0.96191	0.9580
3		0.54042	0.516	0.96180	0.944	1.22443	1.209	1.63429	1.611	2.08931	2.0760
4		0.89833	0.846	1.61624	1.580	2.07309	2.042	2.79610	2.746	3.61033	3.5840
5		1.33229	1.238	2.41101	2.347	3.10924	3.054	4.22674	4.139	5.49950	5.4560
6		1.83895	1.678	3.33639	3.22	4.31991	4.20	5.90872	5.773	7.73528	7.60
7		2.41607	2.17	4.38483	4.22	5.69465	5.54	7.82757		10.29919	10.20
8	3.08253	3.06214	2.71	5.55032	5.32	7.22492	7.02	9.97107		13.17543	13.00
9	3.82966	3.77607	3.36	6.82794	6.51	8.90360	8.63	12.32880		16.34997	16.10
10	4.65087	4.55698		8.21365	7.819	10.72452	10.39	14.89168		19.81072	19.57

IS – present work

NKL – results by Neuhauser, Koonin and Langanke [13]

DHG – results by Demeur, Heenen and Godefroid [16]

$|2p_0\rangle$ – results for states $|2p_0\rangle$ at the points where they are the ground states

Figure 1.

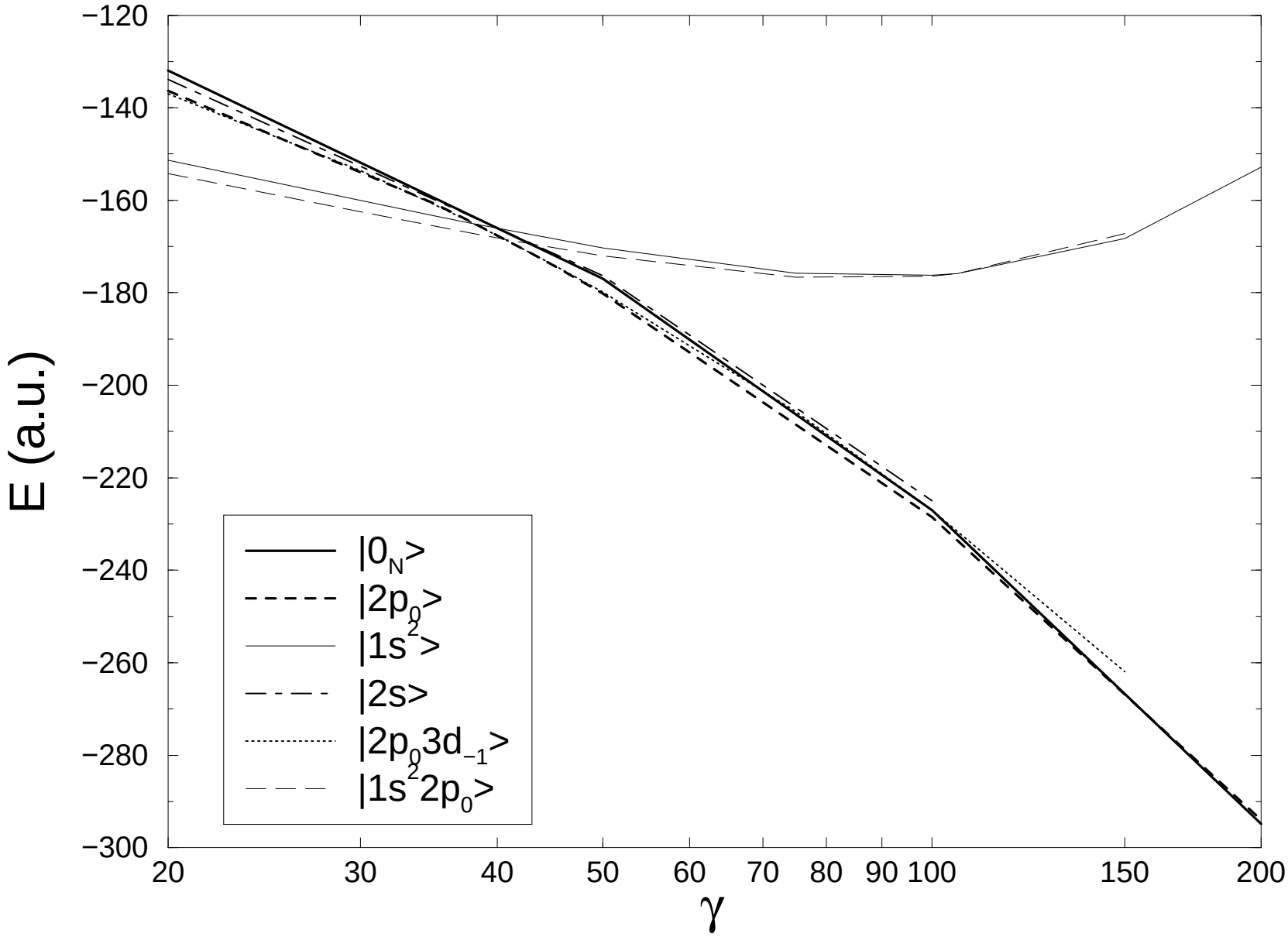

−120
−140
−160
−180
−200
−220
−240
−260
−280
−300
E (a.u.)
20
30
40
50
60
70
80
90
100
150
200
γ
|0N>
|2p0>
|1s2>
|2s>
|2p03d−1>
|1s22p0>

Figure 2

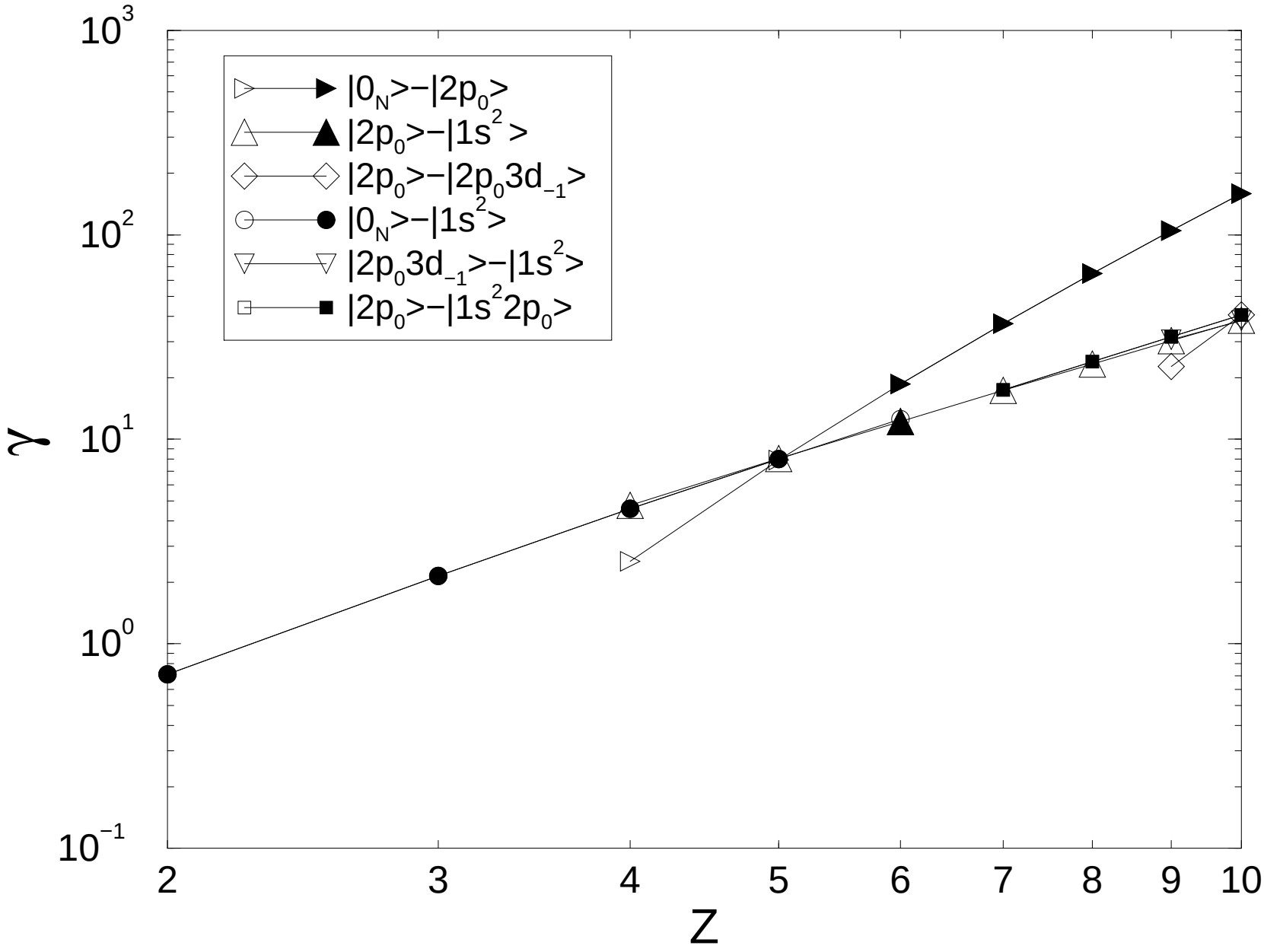

10^3
10^2
10^1
10^0
10^{-1}
γ
2
3
4
5
6
7
8
9
10
Z
$|0_N\rangle - |2p_0\rangle$
$|2p_0\rangle - |1s^2\rangle$
$|2p_0\rangle - |2p_0 3d_{-1}\rangle$
$|0_N\rangle - |1s^2\rangle$
$|2p_0 3d_{-1}\rangle - |1s^2\rangle$
$|2p_0\rangle - |1s^2 2p_0\rangle$

Figure 3

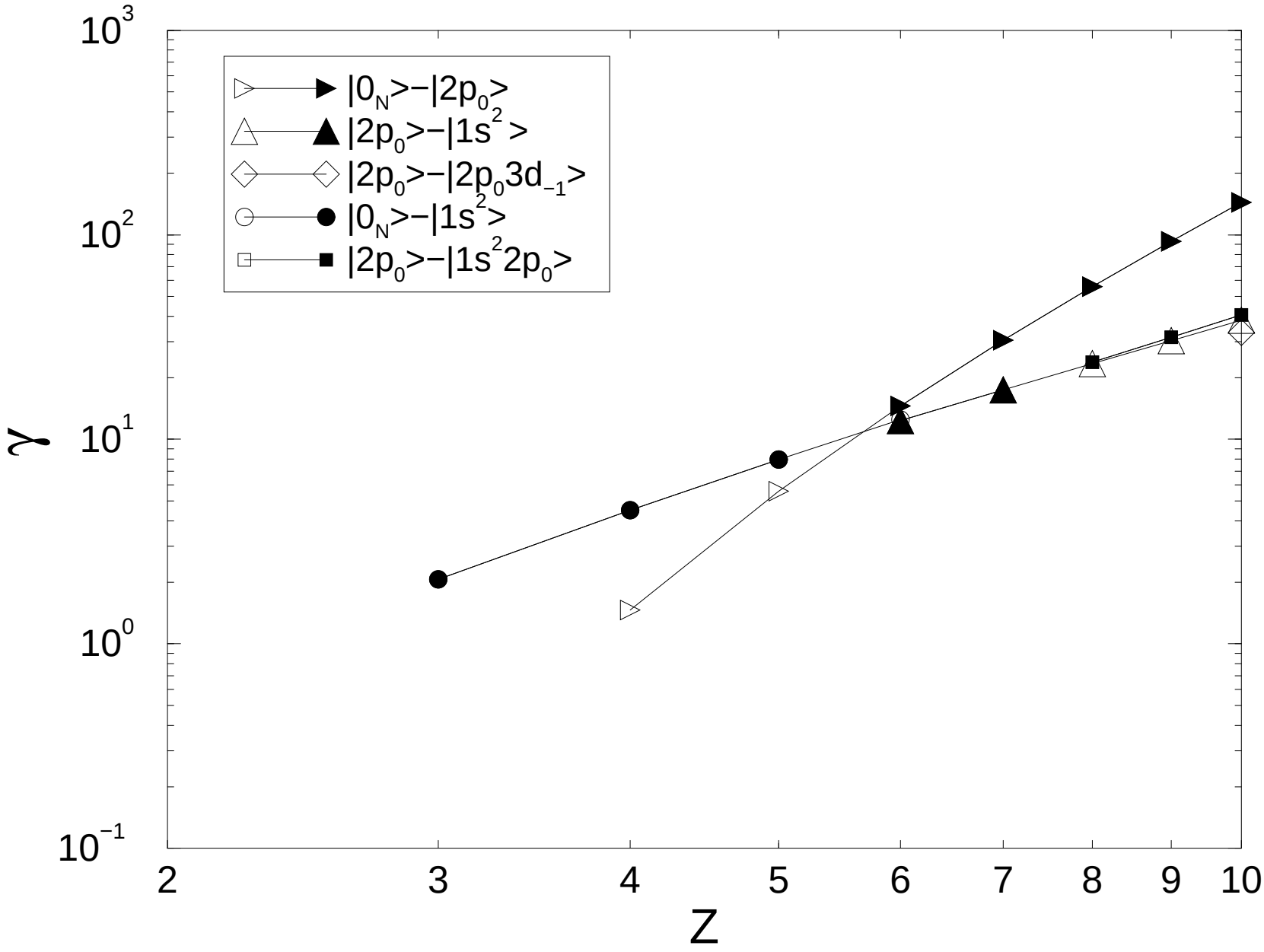

10^3
10^2
10^1
10^0
10^{-1}
γ
2
3
4
5
6
7
8
9
10
Z
$|0_N\rangle - |2p_0\rangle$
$|2p_0\rangle - |1s^2\rangle$
$|2p_0\rangle - |2p_0 3d_{-1}\rangle$
$|0_N\rangle - |1s^2\rangle$
$|2p_0\rangle - |1s^2 2p_0\rangle$

Figure 4

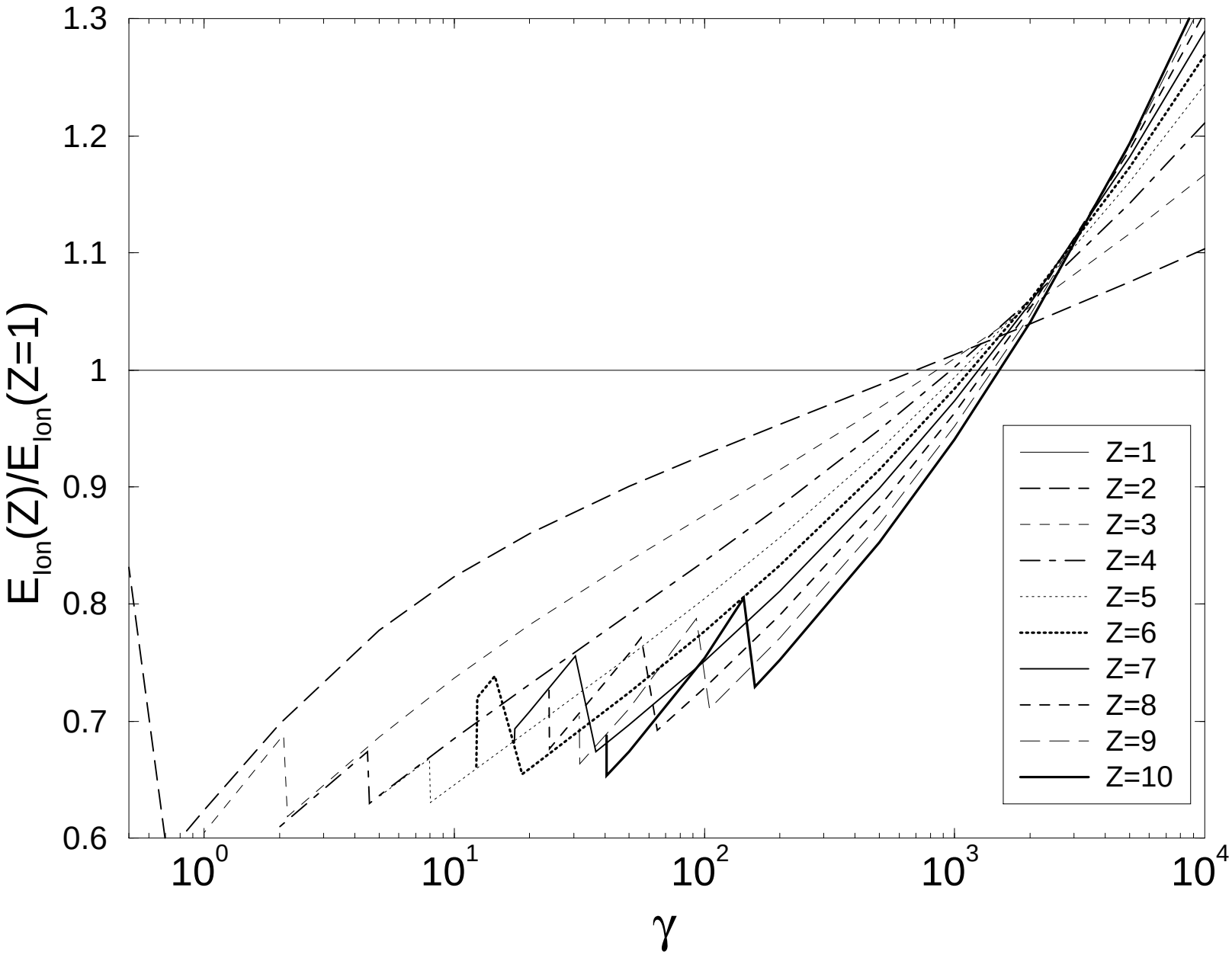
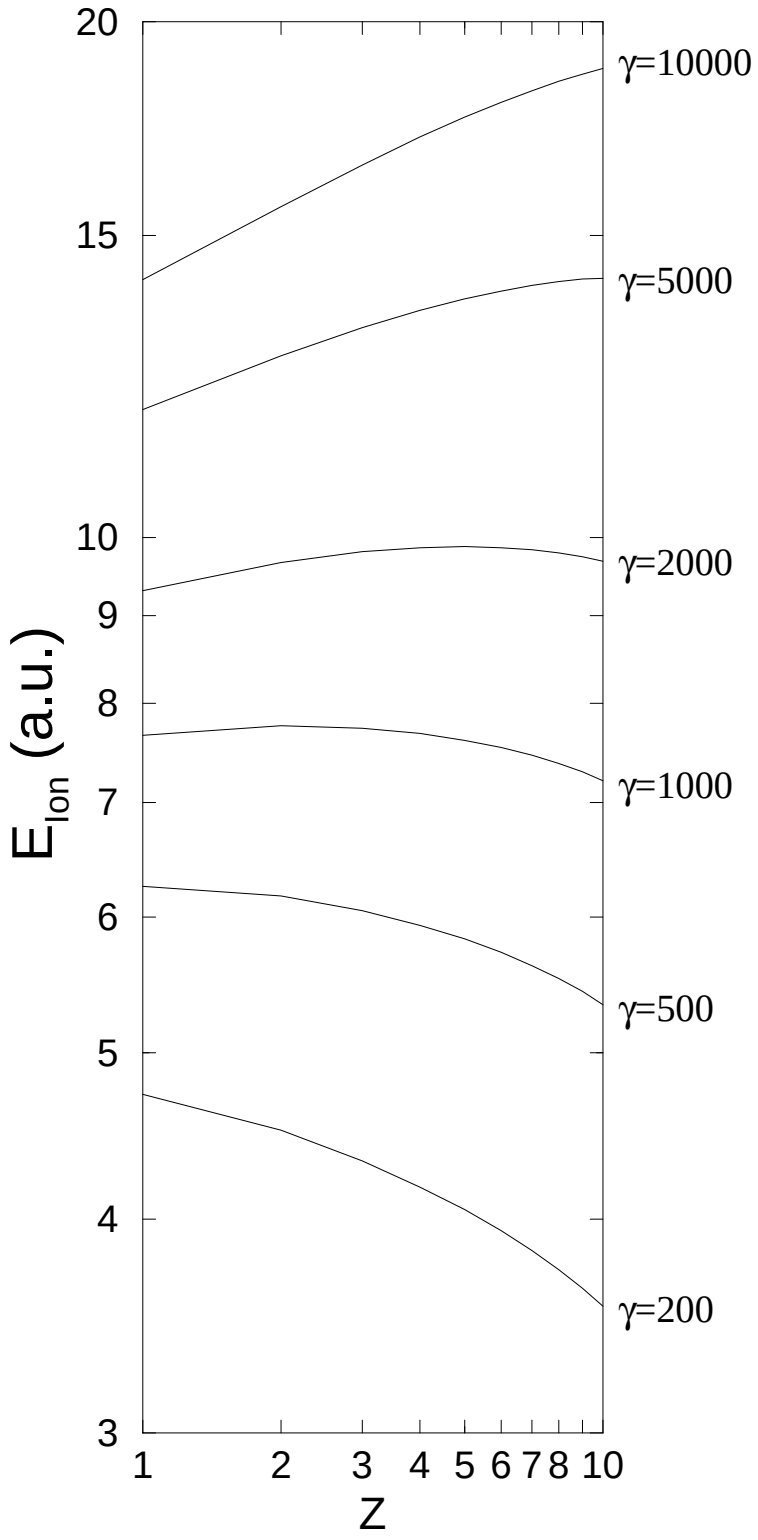

1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
$E_{Ion}(Z)/E_{Ion}(Z=1)$
10^0
10^1
10^2
10^3
10^4
γ
Z=1
Z=2
Z=3
Z=4
Z=5
Z=6
Z=7
Z=8
Z=9
Z=10

Figure 5


20
15
10
9
8
7
6
5
4
3
E_{Ion} (a.u.)
1
2
3
4
5
6
7
8
10
Z
γ=10000
γ=5000
γ=2000
γ=1000
γ=500
γ=200